

# Phloroglucinol, tris(tert-butyldimethylsilyl) ether

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 1,3,5-Benzetriol, 3tbdms derivative   |
| <b>Inchi:</b>               | InChI=1S/C24H48O3Si3/c1-22(2,3)28(10,11)25-19-16-20(26-29(12,13)23(4,5)6)18-21(17,18) |
| <b>InchiKey:</b>            | KBLMIDMVXSUHLD-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C <sub>24</sub> H <sub>48</sub> O <sub>3</sub> Si <sub>3</sub>                        |
| <b>SMILES:</b>              | CC(C)(C)[Si](C)(C)Oc1cc(O[Si](C)(C)C(C)(C)C)cc(O[Si](C)(C)C(C)(C)C)c1                 |
| <b>Mol. weight [g/mol]:</b> | 468.89  |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.26   |      | Crippen Method |
| logp          | 8.839   |      | Crippen Method |
| rinpol        | 2240.80 |      | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U352459&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U352459&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>rinpol:</b>  | Non-polar retention indices         |

Latest version available from:

<https://www.chemeo.com/cid/84-221-3/Phloroglucinol-tris-tert-butyldimethylsilyl-ether.pdf>

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